Dynamic van der Waals Theory : A Phase Field Model of Fluids

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Dynamic van der Waals Theory

A Phase Field Model of Fluids

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In usual theories of phase transitions, the fluctuations of the temperature T are assumed to be small and are neglected. However, there can be situations in which phase transitions occur in inhomogeneous T. For example, wetting properties near the gas-liquid critical point are very sensitive to applied heat flux and boiling processes remain largely unexplored [A. Onuki, *Phase Transition Dynamics* (Cambridge, 2002)]. To treat such problems we propose to start with a coarse-grained entropy rather than a Ginzburg-Landau free energy. For one-component fluids, let an entropy functional $\mathcal{S}$ be determined by the local number density $n = n(\boldsymbol{r}, t)$ and the local internal energy density $e = e(\boldsymbol{r}, t)$ as

$$\mathcal{S} = \int d\boldsymbol{r} \left[ns - \frac{1}{2} C |\nabla n|^2 \right] \tag{1}$$

We assume that $s = s(n, e)$ is the entropy per particle defined as a function of n and e. The gradient term represents a decrease of the entropy due to inhomogeneity of n. We introduce the local temperature $T' = T'(n, e)$ by

$$\frac{1}{T} = \frac{\delta}{\delta e} \mathcal{S} \tag{2}$$

where n is fixed in the derivative. For the special form of Eq.1 we simply obtain $1/T = n(\partial s/\partial e)_n$. Maximization of $\mathcal{S}$ under a fixed total particle number $\int d\boldsymbol{r} n$ and a fixed total energy $\int d\boldsymbol{r} e$ leads to the equilibrium conditions T' =const. and $h/T \equiv \delta \mathcal{S}/\delta n$ =const. As first derived by van der Waals, the equilibrium interface density profile $n = n(x)$ is determined by $h = \mu(n, T') - CTd^2 n/dx^2$ =const. [J.S. Rowlinson, J. Stat. Phys. **20**, 197 (1979)]. In the van der Waals theory $s = s(n, e)$ is given by

$$s = k_{\mathrm{B}} \ln[(e/n + \epsilon v_0 n)^{d/2} (1/v_0 n - 1)] + \text{const.} \tag{3}$$

where v_0 and ϵ are positive constants representing the molecular volume and the magnitude of the attractive potential, respectively, and d is the space dimensionality.

The reversible part of the stress tensor reads

$$\Pi_{ij} = p\delta_{ij} + CT \left[\nabla_i n \nabla_j n - (n\nabla^2 n + |\nabla n|^2/2)\delta_{ij} \right] \tag{4}$$

where $p = n(\mu + sT') - e$ is the van der Waals pressure. The mass density $\rho = mn$ obeys the continuity equation. The momentum density $\boldsymbol{J} = \rho \boldsymbol{v}$ and the energy density obey appropriate dynamic equations

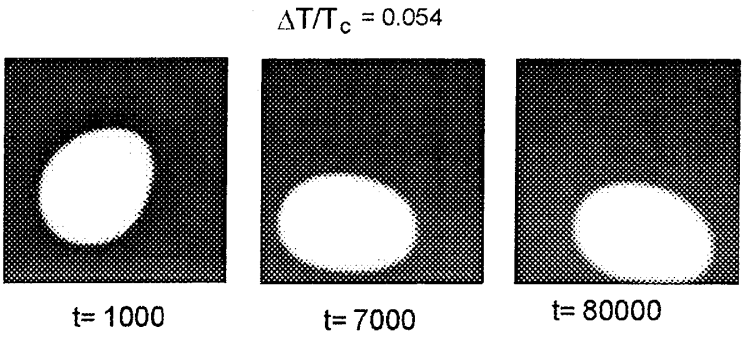

FIG. 1: Migration of a gas droplet towards the heated boundary (bottom) in zero gravity.

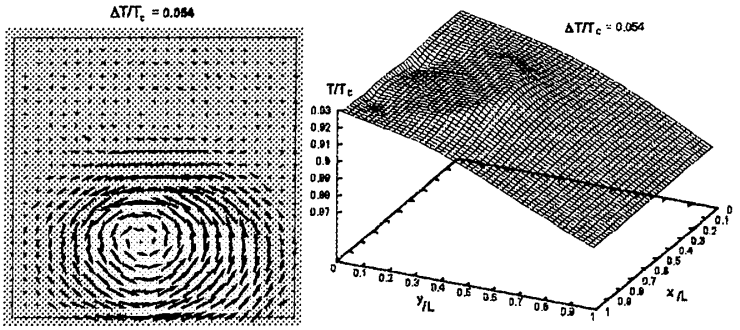

FIG. 2: The velocity field (left) and the temperature (right) in the nearly steady state at $t = 80000$ in Fig.1. There is a velocity component through the interface. The latent heat tranport makes ∇T vanish inside the droplet.

including the gradient part of the stress tensor. The entropy production rate dS/dt within the fluid is non-negative-definite if there is no heat flow from outside.

We give a numerical solution of our phase field model imposing a wetting boundary condition on all the boundaries. At $t =$ we placed a gas droplet at the center of the cell in equilibrium at $T' = 0.875T'_c$. The bottom boundary was then increased by a constant $\Delta T = 0.054T_c$ for $t > 0$, while the top boundary was held at the initial temperature. There is no gravity, while we use "bottom" and "top". Fig.1 shows droplet migration toward the bottom, caused by a Marangoni effect. See a first report: N. O. Young *et al.*, J. Fluid Mech. **6**, 350 (1959) (where bubbles and liquid were different fluids and there was no first-order transition at the interface). Fig.2 displays the velocity and the temperature in the steady state. It is a new finding that the velocity component through the interface is nonvanishing, leading to **latent heat transport**. Because it is highly efficient, a flat temperature or **no temperature gradient** appears inside the droplet. In the steady state the gas droplet apparently wets the bottom partially, while a very thin liquid layer is sandwiched between the bottom boundary and the droplet. We can define an apparent contact angle $\theta_{\rm eff}$, which is a decreasing function of $\Delta T'$. Garrabos *et al.* observed in space that gas spreads on a heated wall initially wetted by liquid and exhibits an apparent contact angle even larger than $\pi/2$ [Phys. Rev. E **64**, 051602 (2001)]. With further increasing $\Delta T'$ the heated wall is completely covered by gas, eventually leading to film boiling in gravity.